

O 45: Oxides and insulators: Adsorption II

Time: Wednesday 11:15–13:00

Location: WIL C307

O 45.1 Wed 11:15 WIL C307

Atomic scale manipulation of single molecules on ultrathin insulating films using an STM — ●INGMAR SWART, TOBIAS SONNLEITNER, and JASCHA REPP — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

On metallic and semiconducting substrates, atoms and molecules can be manipulated controllably on the atomic scale by the tip of a scanning tunnelling microscope (STM) or atomic force microscope (AFM), allowing the creation of nano-engineered structures. In recent years, ultrathin insulating films have been used in STM studies to decrease the electronic coupling between the adsorbate and the underlying substrate. In contrast to manipulation on metal substrates, the use of traditional lateral manipulation modes cannot be successfully applied to molecules on ultrathin insulating films, due to the unfavorable diffusion barrier to binding energy ratio: it is relatively easy to pick the molecule up from the surface with the STM tip compared to successful lateral manipulation. On insulating films, inelastic excitation is relatively efficient due to the increased life-time of the additional charge. Inelastic excitation can result in lateral motion of the molecule. We studied the inelastic excitation for different parameters to gain control over the direction of the lateral motion. By using this new manipulation scheme we can form well-defined and stable structures consisting of several molecules. The mechanical stability of such structures is evidenced by the motion of the entire complex upon excitation.

O 45.2 Wed 11:30 WIL C307

On the influence of molecular symmetry on surface diffusion — TOBIAS SONNLEITNER, INGMAR SWART, ●NIKO PAVLIČEK, ANDREAS PÖLLMANN, and JASCHA REPP — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Symmetries govern many fields of physics and chemistry. In the case of molecules adsorbed on single-crystal surfaces the symmetry of the combined adsorbate-substrate system is decisive for its properties. For example, in spectroscopy symmetry arguments are the basis of many selection rules. However, in diffusion there do not exist such things as selection rules that completely forbid certain diffusion steps. This raises the question how big structural differences that reduce the symmetries have to be, in order to have a significant influence on the surface-potential landscape.

Here, we address the issue of how diffusion of molecules is influenced by the molecular symmetry in a systematic manner using a scanning tunneling microscope. To this end, we investigated π -conjugated molecules for which four symmetry distinct isomers exist on an insulating surface. Despite minute changes in the molecular structure in such a weakly interacting system we find that the surface-potential landscape is governed by the molecular symmetry. Indeed, the four isomers exhibit four distinctly different diffusion patterns, as evidenced by diffusion movies.

O 45.3 Wed 11:45 WIL C307

Determining the Exact Adsorption Configuration of a Chiral Metal-Organic Complex on a Bulk Insulator — ●ALEXANDER SCHWARZ¹, KNUD LÄMMLER¹, TOM TREVETHAN², MATTHEW WATKINS², ALEX SHLUGER², and ROLAND WIESNDANGER¹ — ¹Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany — ²University College London, Gower Street, London WC1E6BT, United Kingdom

Determining the exact position and geometry of an adsorbed molecule is crucial to understand the chemical and physical properties of a particular molecule-surface system. Here we present a high-resolution non-contact atomic force microscopy (NC-AFM) study of Co-Salen, a paramagnetic, low symmetry, chiral Schiff base metal-organic complex, deposited on NaCl(001), a prototypical bulk insulator [1]. The experimental results are compared to theoretical calculations.

By utilizing a metallic tip and resolving individual banana-shaped molecules, while simultaneously obtaining atomic resolution on the substrate, we find that the central Co atoms always sits on top of a Cl ion. This adsorption site is confirmed by theoretical calculations. Moreover, we could identify 16 orientations of the molecule on NaCl(001). The molecule axis is rotated by about $\pm 5^\circ$ away from ei-

ther $\langle 110 \rangle$ - or $\langle 100 \rangle$ -directions. These 16 low energy configurations are also predicted by theory and reflect the fourfold symmetry of the surface as well as the chirality of the molecule.

[1] K. Lämmle, *et al.*, Nano Lett. **10**, 2965 (2010).

O 45.4 Wed 12:00 WIL C307

Ab-initio calculations of the adsorption energy of physisorbed molecules on ionic surfaces — ●BEATE PAULUS, CARSTEN MÜLLER, and LUKAS HAMMERSCHMIDT — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

The standard density functional methods have their difficulties with describing dispersion forces, especially the long-range van der Waals interactions. Therefore there is a need of highly accurate results especially for physisorbed systems. The method of increments [1] provides a tool to calculate the correlation contribution to the adsorption energy at the coupled cluster level. It is based on the expansion of the correlation energy in terms of localized orbital groups, the Hartree-Fock treatment is performed for the extended systems.

Here we want to present the application of open-shell adsorbants like NO and gold atoms on ceria surfaces, and the adsorption of small molecules on magnesium fluorid surfaces.

[1] B. Paulus, Phys. Rep. 2006, 428, 1 (review); C. Müller, B. Herschend, K. Hermansson, B. Paulus, J. Chem. Phys. 2008, 128, 214701., C. Müller, K. Hermansson, B. Paulus, Chem. Phys. 2009, 362, 91., C. Müller, B. Paulus, K. Hermansson, Surf. Science 2009, 603, 2619.

O 45.5 Wed 12:15 WIL C307

Controlling the charge-state of single molecules — INGMAR SWART, ●TOBIAS SONNLEITNER, and JASCHA REPP — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg

The chemical and physical properties of atoms and molecules adsorbed on surfaces are influenced by several factors, such as molecule-substrate and molecule-molecule interactions. In this context, especially the charge state of adsorbates is of great importance, since it governs various properties, such as the spin-state, the interaction with other adsorbates and the substrate. Here, we present an STM study on single molecules adsorbed on an ultrathin NaCl film supported by a Cu surface. The use of an ultrathin insulating NaCl film electronically decouples the molecules from the metallic substrate. The molecules exhibit two states with considerably different conductance, which are associated with two different charge states. This is evidenced by changes in the scattering of the interface state, as well as spectroscopic data. The charge state of a molecule can be controlled by adding or removing a single electron to or from the molecule with the STM tip, analogous to what has previously been shown for individual metal atoms. Most importantly, both states are stable, that is, an additional charge will remain on the molecule until it is removed by a voltage pulse of opposite polarity. We demonstrate how one can generalize the charge state control to other molecules. Furthermore, we demonstrate how the tunneling barrier is modified by the presence of an additional charge with intramolecular resolution.

O 45.6 Wed 12:30 WIL C307

A comparative study of small Si and Sn clusters On MgO Surface: An ab-initio approach — ●SUDIP CHAKRABORTY¹, CHIRANJIB MAJUMDER², and SUBHASH V GHASIS¹ — ¹Department of Electronic Science, University of Pune, Pune-411007, India — ²Chemistry Division, Bhabha Atomic Research Center, Trombay-400085, Maharashtra

One of the essential aspects of the architecture of a surface-based electronic device is that the substrate should preferably be an insulator (wide band gap), which enables more than one electrical contact to the adsorbed species. In this respect, the MgO surface (001) could serve as an excellent model system for exploring nanoscale electronic architectures with its inert and catalytic nature. Here we report the atomic and electronic structures of Silicon and Tin clusters (number of atoms = 1-6, 9) on the Magnesium Oxide (MgO) surface using DFT calculation. The primary focus of this study is to understand the nature of interaction between Si/Sn and MgO substrate, which in turn will affect the geometries and electronic properties of Si/Sn clusters which

are of technological relevance. The results reveal that for both the cases the single Si/Sn atom prefers to be adsorbed on the top of oxygen on the surface and hollow sites. The adsorption mechanism is completely driven by the adsorbed atom interaction with the MgO surface. The shapes of gas phase clusters get distorted on adsorption on the surface. We have also calculated the Projected Density of States (PDOS) from which we can get the hybridization as well as the charge transfer of the total system after adsorption of ad-atoms (Si/Sn).

O 45.7 Wed 12:45 WIL C307

Adsorption of Au and Pd on a hematite surface — •ADAM KIEJNA and TOMASZ PABISIAK — Institute of Experimental Physics, University of Wrocław, Wrocław, Poland

The adsorption of sumonolayer Au and Pd atoms at the two most

stable (0001) surfaces of hematite, one being terminated by oxygen and the other by iron, is studied by spin-density functional theory. The changes in configuration caused by adsorption and the adsorption energy in different sites and for different Au and Pd coverages are investigated. The results show that both Au and Pd bind strongly to hematite surfaces and induce large changes in their geometry. In most stable Au and Pd adsorption sites the adsorbate atoms form three-fold bonds with surface oxygen atoms. The binding is stronger for Pd than Au and for both adsorbates is distinctly stronger at the oxygen-terminated than at the iron-terminated surface. The adsorbate interactions with substrate iron and oxygen atoms and their contributions to bonding are discussed based on the calculated local density of states and the electron charge transfer. The effect of on-site Coulomb interactions is briefly discussed based on the calculations performed within DFT+U scheme.